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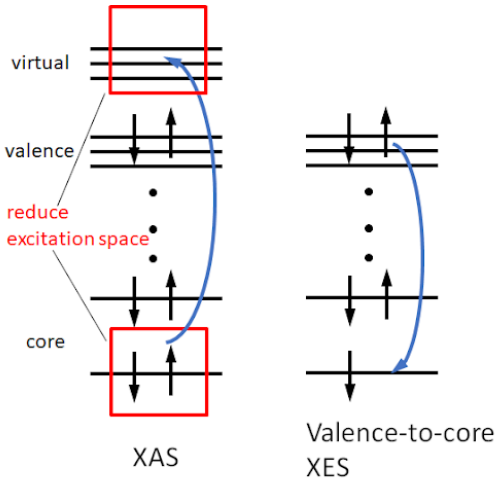
A Quantum Leap Into the Future of Chemistry

Simulating X-ray Absorption and Emission Spectra with TDDFT

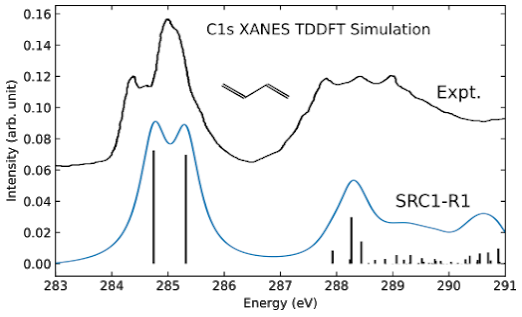


X-ray absorption (XAS) and emission (XES) spectroscopy

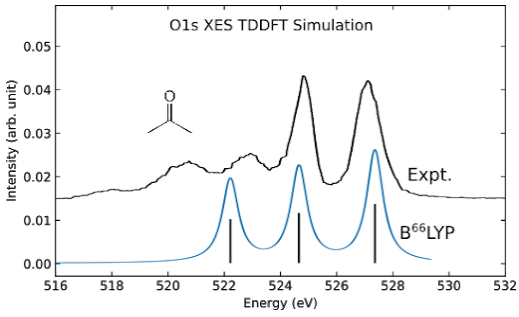
- Difficulty: core-excited states are too high in energy to access through standard bottom-up algorithms for computing excited states.
- Solution: set up a reduced excitation space that includes only relevant core orbitals in the occupied space (as in the core-valence separation scheme).
- Valence-to-core XES transitions are obtained through a TDDFT calculation with a non-Aufbau reference state containing a core hole.

Advantages of using TDDFT for simulating X-ray spectroscopy:

- Good balance between computational accuracy and cost. Can be applied to realistic molecular systems;
- With special-purpose xc functionals (e.g., SRC functionals in Q-Chem), errors in core excitation energies are significantly reduced;
- Only minimal input parameters are necessary (almost).



(a) Simulated XAS for butadiene



(b) Simulated XES for acetone

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